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Intelligent Self-Configuring Client-Server Analysis Software for High-Resolution X and Gamma-Ray Spectrometry

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INTELLIGENT SELF-CONFIGURING CLIENT-SERVER ANALYSIS SOFTWARE FOR HIGH-RESOLUTION X AND GAMMA-RAY SPECTROMETRY

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ABSTRACT

The Safeguards Technology Program at the Lawrence Livermore National Laboratory is developing isotopic analysis software that is constructed to be adaptable to a wide variety of applications and requirements. The MGA++ project will develop an analysis capability based on an architecture consisting of a set of tools that can be configured by an executive to perform a specific task. The software will check the results or progress of an analysis and change assumptions and methodology as required to arrive at an optimum analysis. The software is intended to address analysis needs that arise from material control and accountability, treaty verification, complex reconfiguration and environmental clean-up applications.

INTRODUCTION

Gamma-ray spectrometry is a valuable tool in determining the presence of SNM in a sample. The technique is nondestructive and compliments other measurements such as neutron counting. MGA is the LLNL developed analysis code that is used to determine relative isotopic abundances of primarily Pu isotopes. The code analyzes γ and X-ray spectra taken non-destructively from a sample and through a series of models and calculations determines the isotopic abundances without using external calibrations. Measurements of isotopic abundance can be combined with other non destructive techniques (i.e. calorimetry) to determine total amount for the various Pu isotopes. This combined technique is routinely used for material control and accountability (MC&A).

The current version of MGA works extremely well for samples that are homogeneous and do not contain unusual isotopics. The code has a long track record of providing high quality isotopic data analysis. We have been extending the capabilities of MGA and are presenting, in this paper, an architectural design for our current project.

The rationale for the project is focused on needs presented by new analysis problems and deficiencies in MGA in the areas of maintainability, extendibility and adaptability.

GENERAL DESCRIPTION

MGA++ is expected to perform the functions of MGA, perform them over a wider envelope of isotopics, interferences, sample matrices and counting conditions, and finally perform some analyses not currently performed by MGA. Thus MGA++ would have the capabilities of MGA, $MGAU_9$ for samples enriched in uranium isotopics, $PU238_3$ for samples enriched in ^{238}Pu and mixed metal/oxide capabilities that do not currently exist.

MGA++ will be structured as a tool-box, where the individual modules can be used to form solutions to specific problems.

The performance requirements on MGA++ require reliability and accuracy using MGA as a baseline. They also require ease of modification and enhancement so that the system can address new problems in a timely manner.

One requirement for MGA++ is multiple modes of operation. The code can run in a very automatic mode for operators in the field or fully automatic for unattended applications. It can run in an interactive mode for analysts. It will also run in a highly interactive diagnostic mode for developers.

Software for portable or unattended applications has some different requirements than data acquisition and analysis software designed for laboratory use by scientists. In the field, simplicity and ease of use and calibration are a high priority. Intelligent data acquisition, that quality assures the data in near real-time, and self-diagnosing analysis software improve quick assessment of the adequacy of field measurements.

Operation that makes use of computer controlled multi-channel analyzer (MCA) and analog electronics are necessary for unattended systems, and desirable for most others so that calibration can be automated and the system can adapt easily to changes in the samples or sampling environment.

Current MCA hardware that meets the above requirements include the *InSpector* from Canberra Nuclear Products Group, the *SpectrumMaster 92X*™ and *Nomad*™ from EG&G Ortec, and the *M³CA* from Aquila Technologies / LANL.

All fielded systems benefit from fail-soft operation (no system hangs or application crashes without an automatic restart). This feature is essential for unattended systems. MGA++ will contain fail-soft features and cooperate with watch-dog processes.

Analysis software requirements vary with the application and transparency or other constraints. MGA++ must allow the flexibility of PU600-type[6,7,8] applications.

CLIENT-SERVER ARCHITECTURE

The client-server architecture of MGA++ is a collection of cooperating processes. These processes might all be on the same computer or they might be distributed over a network. The architecture allows a very complex collection of modules and functions to be 'assembled' to address specific tasks quickly and relatively simply. This architecture also allows the individual parts to be simple and independent of other parts of the system.

This model requires support for multi-tasking. This eliminates *MS-DOS*™ and also *Windows*™ as operational computing environments. *Windows 95*™ , *Windows NT*™ , *Unix*™ and *OS/2*™ remain as options for small systems.

Referring to Figure 3, the executive is the controller and primary client. It will communicate with one or more of the other servers listed and can communicate, as well, with other instruments or systems.

The SpecView server implements the graphical user interface and is described elsewhere[1,4]. The executive will not use this server on unattended systems.

The instrument control server is relevant to fixed installations with doors, motors, sensors, and robots that require direction and control. It will not be discussed in detail here. The executive only requires this server if the sensors are persent in the system.

The data collection server provides sample characterization and counting system characterization, in addition to spectral data collection. These two functions provide quality assurance for the data collection process. MGA++ can operate in an 'analysis only' mode that does not require this server.

All three of the above servers could be implemented completely independent of MGA++ for operation in existing proprietary environments.

Software to guide the operator in collecting quality assured (analyzable) data has been developed in the *PRECHECK*[1] function for systems like the Intelligent Isotopic Analysis System (IAAS)[10]. This function allows the operator to determine the suitability of data that will be collected during a short (~1 minute) count where various aspects of the spectra data are checked and an appropriate count time is calculated. The enhanced *PRECHECK* will include examination of dead-time, peak-ratios, resolution and peak shapes. This function can also be called throughout the data collection process to characterize the instrument and assure continued proper operation and analyzable data. In this mode, it would be calculating a dynamic figure-of-merit from the other *PRECHECK* parameters as a barometer of instrument performance.

EXECUTIVE

The MGA++ executive will serve as the controller of the isotopic analysis and manage all interprocess communications between itself and the various servers. It will operate as an inference engine with the rules and knowledge for how isotopic analysis is best performed under various conditions stored in a database of analysis rules and knowledge. If the executive is implemented using a commercial expert system shell, then the rule and knowledge base will reside with that product. If the executive is implemented in a conventional programming language then the rule and knowledge databases will reside with the information manager.

The executive will be the basis for automated analysis under a wide variety of isotopic, sample and counting conditions. Its construction will make the analysis process auditable. This will also allow verification of correct operation of the code.

In its role for managing interprocess communications, it can require authentication and detect tampering of communications. It will use industry standard protocols implemented on flat files, shared memory, network messages or some combination.

Because the methods for performing isotopic analysis reside in the rule and knowledge base, it will be possible to extend MGA++ to solve a much more general class of isotopic analyses than actinide analysis. Applications in environmental monitoring and remediation, hazardous waste characterization and nonproliferation are anticipated.

INFORMATION MANAGER

The information manager will be a server that maintains, delivers and when necessary orders the generation information requested by clients in the MGA++ system.

It will be implemented using the relational model. Since we will not require most of the features and capabilities of a commercial relational database management product, it will probably not rely using a commercial product.

The information manager will manage two distinct databases. The first is a static database that contains gamma-ray information including nuclide, energy, branching intensity and half-lives. It will also contain material absorption data. All data will include reference information so that we will be able to attribute all physical constants and data in the system. This data can not be modified by the information manager, although it can be directed to use a specific database.

The second database will be a dynamic database populated with various data objects required for or generated by the specific analysis in progress.

When a request for information is received by the information manager, the database is checked for the presence and status of the data object. If the object is not present, the information manager looks up what is required to generate the data object, and calls the appropriate routines to perform that function. In a sense, the information manager controls the spectral analysis function of MGA++.

SPECTRAL ANALYSIS METHODOLOGY

The spectral analysis process determines the intensity and energies of the gamma ray photopeaks that have been measured by the detector. After various physical corrections have been applied, these quantities are used to determine the relative isotopic ratios of the radioactive components of the sample.

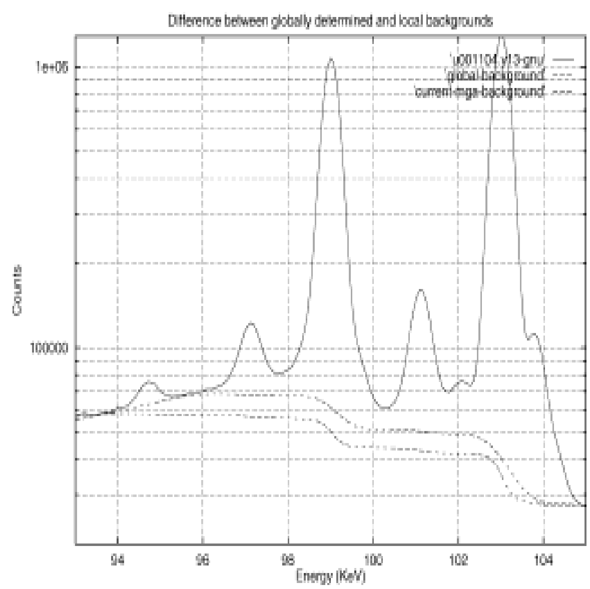

Figure 1. ‘Local’ versus global background determination.

MGA currently uses predetermined windows near a peak or region to determine background. If the isotopics are significantly different than expected or there is an unanticipated interference, this background determination can be significantly in error. We have documented cases where this effect has distorted the results. To solve this problem, we are globally generating background. The effect is illustrated in Figure 1. An example of the automated process is in Figure 2.

The globally determined background is the upper background curve and more appropriately generates the background, especially in the region to the right of 94.66 keV uranium X-ray line.

An automated global background determination will not be dependent on assumptions of relative peak strength and interferences. This will remove one possible source of inaccuracy and potential instability from the analysis.

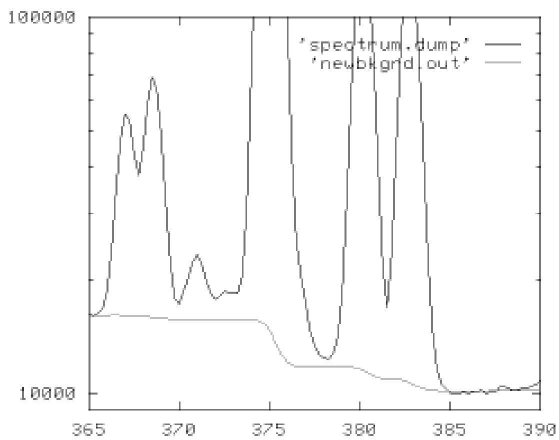

Figure 2. Automated global background determination in the 375 keV region

The background determination is made in three phases. First a global continuum is determined. Next the peak regions are located. Finally a background interpolation is performed in those regions.

The first stage in the spectral analysis process is the determination of the continuum portion of the spectrum. The continuum is primarily due to compton scattered events from both the sample as well as naturally occurring background radiations. Most of the remainder of the spectrum consists of the individual photopeaks corresponding to each gamma ray energy detected. Determination of the continuum is extremely important, especially in the case of low intensity photopeaks as well under multiple peak groupings.

The continuum determination is done in two steps - global and a more precise determination under peak regions. The global process starts with an estimate of the detector resolution parameter; this can be from a calibration of this particular detector or the module will use a generic value as a first guess. The resolution parameter is used to perform a digital filtering operation over the entire spectrum. This is followed with a clipping of all spectral values that exceed a threshold. The resultant spectrum is smoothed and the entire process repeated until a convergent result is achieved.

The global continuum is used to determine regions of potential photopeaks. Each region that contains data exceeding the global continuum are examined, as well as first and second derivatives to confirm that the region seems reasonable as a peak region.

Detailed continuum determination under the peak region is then performed, matching both value and first derivative at the splice points.

The composite continuum is then used for all subsequent analysis of the spectrum.

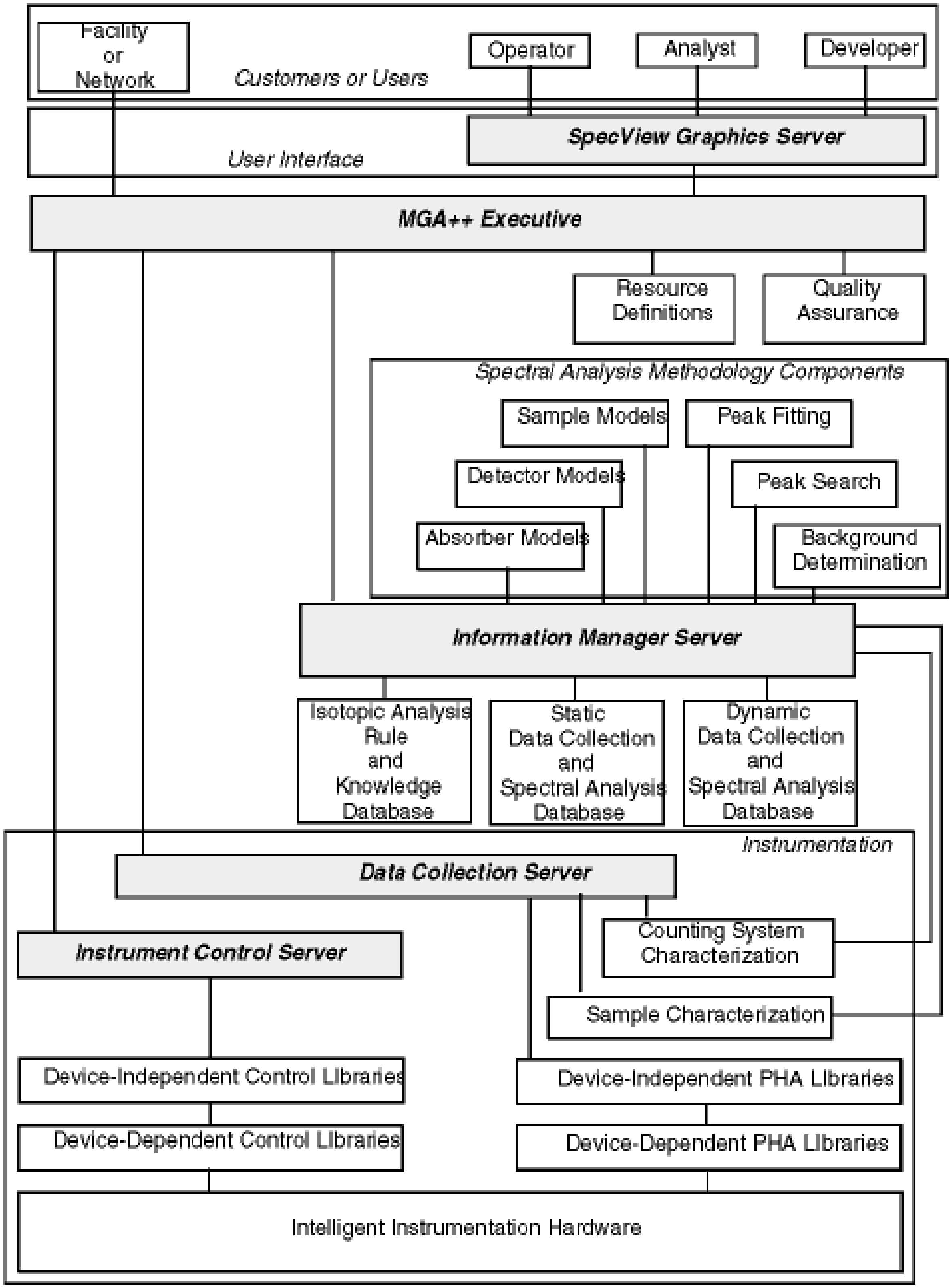

Figure 3. MGA++ Architecture

The process of determining peak regions also provides initial estimates of peak location and height. This information is used to make rough estimates of both isotopic identification and composition. For example, having both 376 keV and 414 keV photopeaks of roughly equal intensity is a reasonable clue that ^{239}Pu might be present in the sample. This would be confirmed by detailed examination of other peaks that should be visible in the spectrum.

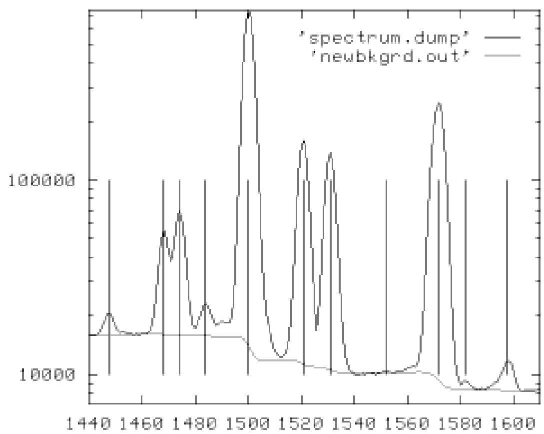

Figure 4. Automated peak search in the 375 keV region

Automated global peak search is desirable to mitigate the same limitations as 'local' background determination. These are isotopic and sample assumptions and unanticipated interferences. An example search in the 375 keV region is shown in Figure 4.

We are currently modifying MGA's absorber model to provide a more analytic solution, again less dependent on assumptions.

We are also providing for multiple detector models so that MGA++ can be used in the analysis of spectra from CdTe, CdZnTe and other medium resolution detectors. Resolution and efficency of these detector systems need to improve before a full isotopic analysis of plutonium is practical.

MGA++ peak fitting methodology will adapt to various peak shapes due to Doppler broadening (x-rays), recoil broadening (n,n',γ), and pile-up. The fitting process will use the Levenberg-Marquardt least-squares method and will be independent of the analytical model of the peak shape.

ONGOING WORK

As an interim product in our project, we are developing an MGA-hi code. This application will perform plutonium and uranium isotopics (including ^{238}Pu) using only spectral data above the 100 keV region. This code will not include an inference engine executive. It will use automatic global background determination and peak region identification. It will also use the physics portion of MGA for its absorbers, sample absorption and detector models. Our performance expectations are 5% accuracy for Pu isotopics and 10% accuracy for U isotopics.

We are also working on a test-bed problem for the inference engine called 'Is it Pu?'.

Because of our 'tool-box' approach, we are approaching commercialization without transferring source code or co-developing software. We will provide an application programming interface (API) to vendors interested in licensing. They will provide the interface that integrates the MGA++ analysis software into their proprietary data collection and viewing environment. They would provide their own user interface to the operation of MGA++. This is being pursued through determining interest and generating memoranda of agreement with the interested vendors. This way we will retain control of the technology to simplify both enhancements and 'in-depth' technical support issues.

We will continue development of verification analysis software, such as our NELA[5] or PU600[6,7,8] codes while MGA++ is under development. We will use as much methodology and domain knowledge from these codes as possible in developing the rule and knowledge bases for MGA++.

SUMMARY

We see a need for advanced analysis software such as *MGA++* that facilitates analysis of a wide variety of samples and sampling conditions. The architecture of MGA++ will allow us to generate isotopic analysis solutions to problems in environmental monitoring and remediation, hazardous waste, nonproliferation and MC&A. Combined with cryo-cooler technology for high-purity germanium detectors, we can address a wider domain of problems in disarmament, emergency response and counter-proliferation.

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